

(FILE 'HOME' ENTERED AT 14:26:16 ON 02 DEC 2003)

FILE 'REGISTRY' ENTERED AT 14:26:22 ON 02 DEC 2003

L1 0 S CL-20/CN
 L2 0 S CL20/CN
 L3 15 S CL-20
 L4 1 S L3 AND HEXA

FILE 'CAPLUS' ENTERED AT 14:28:23 ON 02 DEC 2003

L5 333 S L4
 L6 56 S L5 AND EPSILON
 L7 66714 S INVERSE
 L8 1 S L6 AND L7
 L9 9 S L6 AND CRYSTALLIZATION/IT

FILE 'REGISTRY' ENTERED AT 14:33:31 ON 02 DEC 2003

FILE 'CAPLUS' ENTERED AT 14:34:13 ON 02 DEC 2003

=> s 16 not 19
 L10 47 L6 NOT L9

 => d ibib abs hitstr 19 1-9

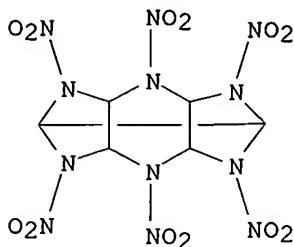
D9 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 2003:532386 CAPLUS
 DOCUMENT NUMBER: 139:87406
 TITLE: Inverse solvent-nonsolvent crystallization of HNIW
 (explosive)
 INVENTOR(S): Hamilton, R. Scott
 PATENT ASSIGNEE(S): USA
 SOURCE: U.S. Pat. Appl. Publ., 8 pp.
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|-----------------|----------|
| US 2003130503 | A1 | 20030710 | US 2002-42522 | 20020109 |
| EP 1327633 | A1 | 20030716 | EP 2003-250026 | 20030106 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK | | | | |
| JP 2003212876 | A2 | 20030730 | JP 2003-3320 | 20030109 |

PRIORITY APPLN. INFO.: US 2002-42522 A 20020109

AB Inverse crystn. of the .epsilon.-polymorph of
 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazatetracyclo[5.5.0.05,903,11]
 (HNIW or CL-20) is carried out by adding CL-20 to a dry solvent and adding
 the CL-20-contg. soln. to a non-solvent, which ppts. out the desired CL-20
 polymorph. A basic salt is typically added to neutralize acidic species
 prior to crystn. Suitable crystn. solvents include Et acetate, Me
 acetate, iso-Pr acetate, Bu acetate, THF, and Me Et ketone; suitable
 crystn. non-solvents include hexane, cycloheptane, heptane, octane,
 benzene, toluene, and xylene. CL-20 is preferably synthesized by
 nitration of 2,6,8,12-tetraacetyl-2,4,6,8,10,12-

hexaazatetracyclo[5.5.0.05,903,11] (TADA).
 IT 135285-90-4P
 RL: IMF (Industrial manufacture); PRP (Properties); PUR (Purification or recovery); PREP (Preparation)
 (inverse solvent-nonsolvent crystn. of HNIW (explosive))
 RN 135285-90-4 CAPLUS
 CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



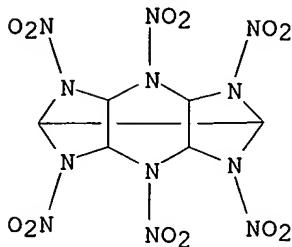
~~ANSWER 2 OF 9~~ CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 2002:153686 CAPLUS
 DOCUMENT NUMBER: 136:202705
 TITLE: Crystallization of 2,4,6,8,10,12-hexanitro-
 2,4,6,8,10,12-hexaazatetracyclo[5.5.0.05,903,11]-
 dodecane-an organic oxidizer used as energetic filler
 in weapons
 INVENTOR(S): Sanderson, Andrew J.; Hamilton, Richard S.; Warner,
 Kirstin F.
 PATENT ASSIGNEE(S): Alliant Techsystems Inc., USA
 SOURCE: U.S., 6 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|---|----------|---|------------|
| US 6350871 | B1 | 20020226 | US 2001-813687 | 20010321 |
| PRIORITY APPLN. INFO.: | | | US 2000-193468P | P 20000331 |
| AB | 2,4,6,8,10,12-Hexanitro-2,4,6,8,10,12-hexaazatetracyclo[5.5.0.05,903,11]-dodecane (CL-20) is crystd. by dissolving CL-20 in an org. solvent to form a satd. soln., adding a nitrate ester, in which CL-20 is not sol. but which is miscible with the org. solvent, at a nitrate ester to CL-20 wt. ratio of (5-8):1, adding cryst. seeds of the .epsilon.-polymorph of CL-20 to the satd. soln., evapg. the solvent at 25-60.degree.C while growing CL-20 crystals, and removing the nitrate ester and residual solvent from the crystals. The nitrate ester can be poly(glycidyl nitrate), triethyleneglycol-dinitrate, butanetrioltrinitrate, or diglycerol tetranitrate. The org. solvent is preferably Et acetate, but a ketone, a cyclic ether, nitromethane, or acetonitrile can also be used. CL-20 is an org. oxidizer used as energetic filler in weapons. | | | |
| IT | 135285-90-4P | | RL: NUU (Other use, unclassified); PEP (Physical, engineering or chemical | |

process); PUR (Purification or recovery); PYP (Physical process); PREP (Preparation); PROC (Process); USES (Uses)
 (crystn. of, oxidizer; crystn. of
 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazatetracyclo[5.5.0.05,903,11
]-dodecane-an org. oxidizer used as energetic filler in weapons)

RN 135285-90-4 CAPLUS

CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 3 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1999:747438 CAPLUS

DOCUMENT NUMBER: 132:4554

TITLE: Crystallization of explosive hexanitrohexaazaisowurtzitane (HNIW) using .
 epsilon.-HNIW as seed crystals

INVENTOR(S): Kawabe, Hidefumi; Miya, Hiroshi

PATENT ASSIGNEE(S): Asahi Chemical Industry Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.

DOCUMENT TYPE: Patent

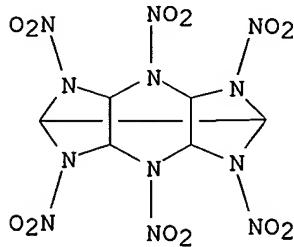
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|---|----------|-----------------|----------|
| JP 11322752 | A2 | 19991124 | JP 1998-148290 | 19980514 |
| PRIORITY APPLN. INFO.: | | | JP 1998-148290 | 19980514 |
| AB | In the manuf. of high-d., high-energy, and high-purity .epsilon.-HNIW from .alpha.-HNIW, .beta.-HNIW, or .gamma.-HNIW by crystn., the starting material is dissolved in a mixed solvent contg. good solvent and poor solvent (whose b.p. is 20.degree. higher than the good solvent), adding .epsilon.-HNIW crystals into the soln., dropping poor solvent into the soln., and forming .epsilon.-HNIW by evapg. the solvent. The good solvent is selected from acetone, methylethylketone, THF, and Et acetate, and the poor solvent is selected from toluene and xylene. The .epsilon.-HNIW is used in the manuf. of explosives. | | | |
| IT | 135285-90-4P, 2,4,6,8,10,12-Hexanitrohexaazaisowurtzitane | | | |
| | RL: PEP (Physical, engineering or chemical process); PRP (Properties); PUR (Purification or recovery); PREP (Preparation); PROC (Process) | | | |
| | (.epsilon.-form; crystn. of explosive hexanitrohexaazaisowurtzitane using .epsilon.-HNIW as seed | | | |

crystals)
 RN 135285-90-4 CAPLUS
 CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



~~D9~~ ANSWER 4 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1999:292584 CAPLUS
 DOCUMENT NUMBER: 130:298968
 TITLE: Antisolvent-solvent crystallization of hexanitrohexaazaisowurtzitane to obtain the .
 epsilon.-polymorph
 INVENTOR(S): Bescond, Philippe; Graindorge, Herve; Mace, Helene
 PATENT ASSIGNEE(S): Societe Nationale des Poudres et Explosifs, Fr.
 SOURCE: Eur. Pat. Appl., 12 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: French
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|-----------------|----------|
| EP 913374 | A1 | 19990506 | EP 1998-402636 | 19981023 |
| EP 913374 | B1 | 20020130 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | | |
| FR 2770216 | A1 | 19990430 | FR 1997-13546 | 19971029 |
| FR 2770216 | B1 | 19991203 | | |
| US 5973149 | A | 19991026 | US 1998-168413 | 19981008 |
| NO 9805000 | A | 19990430 | NO 1998-5000 | 19981027 |
| JP 2000128685 | A2 | 20000509 | JP 1998-346525 | 19981029 |

PRIORITY APPLN. INFO.: FR 1997-13546 A 19971029

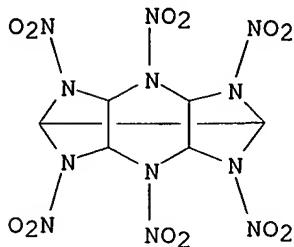
AB A crystn. process for obtaining the .epsilon.-polymorph of HNIW (hexanitrohexaazaisowurtzitane) is carried out by: (1) prep. a satd. soln. of mixed-crystal-morphol. HNIW contg. an org. solvent, selected from a group consisting of esters, nitriles, ethers, and ketones (excluding acetone), and their mixts., and a non-solvent, selected from aliph. and arom. hydrocarbons, and their mixts., in which the solvent for HNIW is more volatile than the non-solvent, (2) seeding the satd. crystal soln. with crystals of the .epsilon.-polymorph of HNIW, and (3) concn. of the soln. by evapn., preferably at <50.degree.. The esters are preferably formates and acetates, typically Me acetate, Et acetate, iso-Pr acetate; preferred arom. hydrocarbons are xylenes and toluene.

IT 135285-90-4P, Hexanitrohexaazaisowurtzitane

RL: IMF (Industrial manufacture); PUR (Purification or recovery); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses) (antisolvent-solvent *crystn.* of hexanitrohexaazaisowurtzitane to obtain the *epsilon*-polymorph)

RN 135285-90-4 CAPLUS

CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1999:130417 CAPLUS

DOCUMENT NUMBER: 130:184546

TITLE: Use of chlorine-free non-solvents in solvent-crystallization of 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12,-hexaazatetracyclo [5.5.0.05,9.03,11]-dodecane (CL-20) explosive

INVENTOR(S): Johnston, Harold Eugene; Wardle, Robert B.

PATENT ASSIGNEE(S): Cordant Technologies Inc., USA

SOURCE: U.S., 8 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

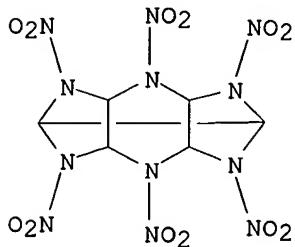
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|-----------------|----------|
| US 5874574 | A | 19990223 | US 1997-991432 | 19971216 |
| PRIORITY APPLN. INFO.: | | | US 1997-991432 | 19971216 |
| AB The high-d. <i>epsilon</i> -polymorph of cryst. CL-20 (explosive) [2,4,6,8,10,12-hexanitro-2,4,6,8,10,12,-hexaazatetracyclo [5.5.0.05,9.03,11]-dodecane] is isolated by: (1) drying a water-contg. soln. of CL-20 in a solvent, (2) adding a low-d. chlorine-free non-solvent for CL-20 to the dry solvent soln. to induce crystn. and pptn. of the <i>epsilon</i> -polymorph, (3) sepg. the pptd. <i>epsilon</i> -CL-20 by adding a polar dense solvent (preferably water) to displace the non-solvent and solvent from the surface of the CL-20 crystals, and (4) recovering the wet CL-20 crystals. An inorg. base can be added to the initial soln. to neutralize any acidic compds. prior to crystn. In addn., a quantity of <i>epsilon</i> -polymorph CL-20 is added as crystn. seeds. The solvent is chosen from Et acetate, Me acetate, iso-Pr acetate, Bu acetate, THF, and MEK. The chlorine-free non-solvent is typically a hydrocarbon chosen from hexane, cyclohexane, heptane, octane, benzene, | | | | |

toluene, xylene, hydrocarbon oils, petroleum ether, and ligroine. In this fashion, the *epsilon*-polymorph CL-20 is made wet for later handling, packaging, and shipping.

IT 135285-90-4P, 2,4,6,8,10,12-Hexanitro-2,4,6,8,10,12,-hexaazatetracyclo [5.5.0.05,9.03,11]-dodecane
 RL: IMF (Industrial manufacture); PUR (Purification or recovery); PREP (Preparation)
 (use of chlorine-free non-solvents in solvent crystn. of 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12,-hexaazatetracyclo [5.5.0.05,9.03,11]-dodecane (CL-20) explosive)

RN 135285-90-4 CAPLUS

CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

~~ANSWER 6 OF 9~~ CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1998:697125 CAPLUS
 DOCUMENT NUMBER: 129:316246
 TITLE: Preparation of *epsilon*-hexanitrohexaazaisowurtzitane as an explosive
 INVENTOR(S): Kawanabe, Shushi; Miya, Hiroshi
 PATENT ASSIGNEE(S): Asahi Chemical Industry Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-------------|------|----------|-----------------|----------|
| JP 10287674 | A2 | 19981027 | JP 1997-111756 | 19970415 |
| JP 2779614 | B2 | 19980723 | | |

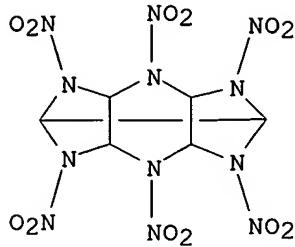
PRIORITY APPLN. INFO.: JP 1997-111756 19970415

AB Title compd. (*epsilon*-I), useful as an explosive (no data), is prep'd. by dissolving I into low-boiling good solvent-poor solvent mixts. and evapg. for crystn. *alpha*-I in Me₂CO was mixed with xylene and evapd. to give 92.0% *epsilon*-I.

IT 135285-90-4, Hexanitrohexaazaisowurtzitane
 RL: PEP (Physical, engineering or chemical process); PROC (Process)
 (prep'n. of *epsilon*-hexanitrohexaazaisowurtzitane by
 crystn. from low-boiling solvent mixts.)

RN 135285-90-4 CAPLUS

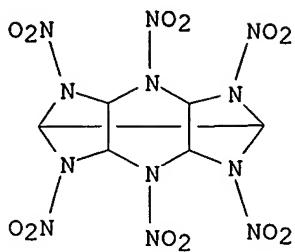
CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



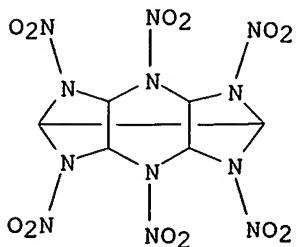
~~ANSWER 7 OF 9~~ CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1998:693443 CAPLUS
 DOCUMENT NUMBER: 129:316245
 TITLE: Preparation of *epsilon*-hexanitrohexaazaisowurtzitane using seed crystal
 INVENTOR(S): Kawabe, Hidefumi; Miya, Hiroshi
 PATENT ASSIGNEE(S): Asahi Chemical Industry Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

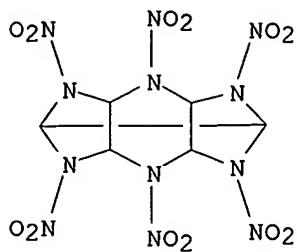
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-------------|------|----------|-----------------|----------|
| JP 10287675 | A2 | 19981027 | JP 1997-111757 | 19970415 |
| JP 2893524 | B2 | 19990524 | | |

PRIORITY APPLN. INFO.: JP 1997-111757 19970415
 AB Title compd. (*epsilon*-I), useful as an explosive (no data), is
 prep'd. by dissolving I into low-boiling good solvent-poor solvent mixts.,
 mixing with *epsilon*-I seed crystal, and evapg. for crystn.
alpha-I in Me₂CO was mixed with PhMe and *epsilon*-I seed
 crystal and evapd. at 3.0-4.0 wt.-%/h to give 98.0% *epsilon*-I.
 IT 135285-90-4, Hexanitrohexaazaisowurtzitane
 RL: PEP (Physical, engineering or chemical process); PROC (Process)
 (prepn. of *epsilon*-hexanitrohexaazaisowurtzitane by
 crystn. using seed crystal)
 RN 135285-90-4 CAPLUS
 CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



~~ANSWER 8 OF 9~~ CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1998:440700 CAPLUS
 DOCUMENT NUMBER: 129:110953
 TITLE: Crystallization behavior of hexanitrohexaazaisowurtzitane at 298 K and quantitative analysis of mixtures of its polymorphs by FTIR
 AUTHOR(S): Kim, Jun-Hyung; Park, Young-Chul; Yim, Yoo-Jin; Han, Jeong-Sik
 CORPORATE SOURCE: Agency for Defense Development, Taejon, 305-600, S. Korea
 SOURCE: Journal of Chemical Engineering of Japan (1998), 31(3), 478-481
 CODEN: JCEJAQ; ISSN: 0021-9592
 PUBLISHER: Society of Chemical Engineers, Japan
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The crystn. behavior of hexanitrohexaazaisowurtzitane (HNIW) has been investigated at 298 K. Only the .beta. form crystd. at the initial stage of crystn., and it converted to the .epsilon. form with a soln.-mediated transformation mechanism. Through the measurement of the solubilities of each polymorph (.beta. and .epsilon.) at 298 K, it was confirmed that the .epsilon. form is stable and the .beta. form is metastable. In addn., an anal. method has been developed for the detn. of the fraction of the .epsilon. form in the ppts. using a FTIR spectrometer.
 IT 135285-90-4, Hexanitrohexaazaisowurtzitane
 RL: PEP (Physical, engineering or chemical process); PRP (Properties);
 PROC (Process)
 (CL-20; crystn. of hexanitrohexaazaisowurtzitane at 298 K and FTIR anal. of its polymorphs)
 RN 135285-90-4 CAPLUS
 CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)





REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1998:424235 CAPLUS
 DOCUMENT NUMBER: 129:110410
 TITLE: Salting-out process of crystallizing 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazatetracyclo[5.5.0.05,903,11]dodecane (CL-20)
 INVENTOR(S): Johnston, H. Eugene; Wardle, Robert B.
 PATENT ASSIGNEE(S): Thiokol Corp., USA; Johnston, H. Eugene; Wardle, Robert B.
 SOURCE: PCT Int. Appl., 33 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|------------|
| WO 9827072 | A1 | 19980625 | WO 1997-US22298 | 19971212 |
| W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, FI, GB, GE, GH, GM, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG | | | | |
| AU 9853743 | A1 | 19980715 | AU 1998-53743 | 19971212 |
| EP 946527 | A1 | 19991006 | EP 1997-950849 | 19971212 |
| R: CH, DE, FR, GB, LI, SE | | | | |
| JP 2001510465 | T2 | 20010731 | JP 1998-527767 | 19971212 |
| NO 9902929 | A | 19990616 | NO 1999-2929 | 19990616 |
| PRIORITY APPLN. INFO.: | | | US 1996-33392P | P 19961217 |
| | | | WO 1997-US22298 | W 19971212 |

AB In the process, CL-20 is dissolved in a mixt. of H2O and a solvent for CL-20, e.g., EtOAc, to form 2 liq. phases comprising H2O and wet solvent contg. CL-20. The phases are sepd., the CL-20 soln. in the wet solvent is dried by azeotropic distn., a base, e.g., Na2CO3 is added to the dry CL-20 soln. to neutralize acidic species, and a low-d., CL-20 nonsolvent is added to the resulting CL-20 soln. to cause pptn. of *epsilon*-polymorph CL-20. The CL-20 crystals are sepd. from the nonsolvent and the solvent by adding sufficient H2O to displace the nonsolvent and the solvent from the surface of the CL-20 crystals. In this fashion, the .

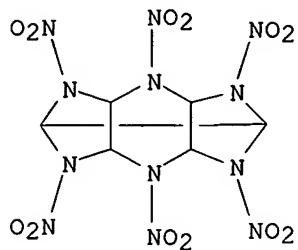
epsilon-polymorph CL-20 is made wet for later handling, packaging, and shipping. A schematic presentation of the app. for the process is included.

IT 135285-90-4P, CL-20

RL: PUR (Purification or recovery); PREP (Preparation)
(**epsilon**-polymorph; salting-out process of crystg.
2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazatetracyclo[5.5.0.05,903,11
]dodecane)

RN 135285-90-4 CAPLUS

CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-
hexanitro- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

9

THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/042,522

=> d ibib abs hitstr 110 1-47

L10 ANSWER 1 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2003:718354 CAPLUS
DOCUMENT NUMBER: 139:325475

TITLE: Voids and density distributions in 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexazaisowurtzitane (CL-20) prepared under various conditions

AUTHOR(S): Hoffman, D. Mark
CORPORATE SOURCE: Energetic Materials Center, Lawrence Livermore National Laboratory, Livermore, CA, 94551, USA
SOURCE: Propellants, Explosives, Pyrotechnics (2003), 28(4), 194-200

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English

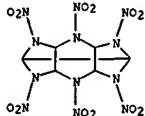
AB The d. distributions of six samples of CL-20 were measured by using the d. gradient technique. The technique was used to det. which prep. procedure produced the highest av. CL-20 d. Assuming crystals with fewer flaws result in reduced sensitivity to shock initiation, higher av. crystal d. (closest to the theor. max. d.) would imply the least no. of voids or inclusions. Based on hot-spot theory, better crystals, i.e., smaller no. of flaws will reduce the shock sensitivity and perhaps other impact initiation mechanisms as well. Six samples from different synthesis and crystal procedures gave av. densities from 2.042-2.023 g/cm³ as measured by d. gradient. Assuming the voids have no d., the crystals were between 99.90-99.98% of the theor. max. d. (TM for epsilon CL-20 is 2.044 g/cm³). An attempt was made to account for the d. difference by identifying voids in the crystals by using polarized light microscopy. This method also gave some insight into the different morphologies produced by different cryst. techniques. In 3 cases voids on the order of several micrometers can be resolved in large CL-20 crystals.

IT 135285-90-4P, CL-20

RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses); (voids and d. distributions in 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexazaisowurtzitane explosive prep. under various conditions)

RN 135285-90-4 CAPLUS

CN 5,2,6-(iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 1 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

L10 ANSWER 2 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2003:284116 CAPLUS
DOCUMENT NUMBER: 138:306227

TITLE: Synthesis of epsilon polymorphic form of a isowurtzitane derivative for explosives and pyrotechnic compositions
INVENTOR(S): Cagnon, Guy; Jacob, Guy; Mace, Helene
PATENT ASSIGNEE(S): Societe Nationale des Poudres et Explosifs SNPE, Fr.
SOURCE: Fr. Demande, 15 pp.
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-------------|------|----------|------------------|----------|
| FR 2830533 | A1 | 20030411 | FR 1996-3209 | 19960314 |
| NL 1005411 | C2 | 20030516 | NL 1997-1005411 | 19970303 |
| DE 19710189 | A1 | 20030703 | DE 1997-19710189 | 19970312 |
| ES 2191501 | A1 | 20030901 | ES 1997-548 | 19970313 |

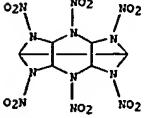
PRIORITY APPN. INFO.: FR 1996-3209 A 19960314

AB The invention relates to polymorphic epsilon -hexanitrohexaazaisowurtzitane and its synthesis. According to a 1st variant, hexanitrohexaazaisowurtzitane of an unspecified polymorphic form is made in a premixt. contg. 20-40 glycidyl polyazoture and 60-80 wt.% of gtorc₁ trinitrate of a monomeric triol contg. 3-12 C atoms. The mixt. is heated in gtorc₁ cycle at 40-60 degrees, and then at 10-30 degrees, and components from the premixt. are eliminated by washing with an org. solvent. According to a 2nd variant, a satd. soln. of hexanitrohexaazaisowurtzitane of an unspecified polymorphic form in an acetone-toluene mixt. is prep'd., the soln. is seeded with several crystals of epsilon-hexanitrohexaazaisowurtzitane, and the soln. is concd. by evapn. of acetone. Hexanitrohexaazaisowurtzitane, in particular a dense epsilon-form, is suitable for explosives or an oxidizing agent used in pyrotechnic compns.

IT 135285-90-4P, Hexanitrohexaazaisowurtzitane
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PNU (Preparation, unclassified); PREP (Preparation); PROC (Process)
(synthesis of epsilon-hexanitrohexaazaisowurtzitane for explosives and pyrotechnic compns.)

RN 135285-90-4 CAPLUS

CN 5,2,6-(iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



L10 ANSWER 3 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2003:117774 CAPLUS
DOCUMENT NUMBER: 138:172811

TITLE: Low-sensitivity explosives containing CL-20 and plasticized energetic binder
INVENTOR(S): Lee, Kenneth E.; Braithwaite, Paul C.; Nicolich, Steve; Mezger, Mark

PATENT ASSIGNEE(S): Alliant Techsystems Inc., USA
SOURCE: PCT Int. Appl., 28 pp.

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|-----------|-----------------|----------|
| WO 2003011797 | A2 | 20030213 | WO 2002-US24349 | 20020731 |
| WO 2003011797 | A3 | 200303424 | | |
| W: AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, C2, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AH, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RV: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, C2, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |

US 2003094224 A1 20030522 US 2002-210863 20020731

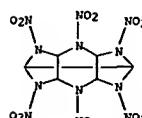
PRIORITY APPN. INFO.: US 2001-309386P P 20010801
AB A low-sensitivity explosive compn. contains 85-96 wt.% HNIW (CL-20) with av. particle size <30 .mu.m (preferably 1-4 .mu.m) and 4-15 wt.% of a plasticized binder, comprised of cellulose acetate butyrate and bis(dinitropropyl) acetal/bis(dinitropropyl) formal (BDNPAP/F). The explosive has a shock sensitivity of <140 cards, as measured by the NOL Card Gap Test. The prepn. method (i.e., the water/solvent slurry method) is designed to retain and maximize the epsilon-CL-20 polymorph.

IT 135285-90-4, CL-20
RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses)

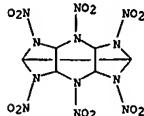
(explosives contg.; low-sensitivity explosives contg. CL-20 and plasticized energetic binder)

RN 135285-90-4 CAPLUS

CN 5,2,6-(iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)

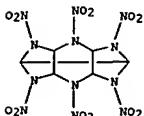


L10 ANSWER 4 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 2002:922797 CAPLUS
 DOCUMENT NUMBER: 138:240068
 TITLE: Ageing and service time period assessment of novel solid rocket propellant formulations containing . epsilon.-CL20, AP and energetic plasticizers
 AUTHOR(S): Bohn, Manfred A.
 CORPORATE SOURCE: Fraunhofer-Institut fuer Chemische Technologie, Pfingstal-Berghausen, D-76318, Germany
 SOURCE: Proceedings of the International Pyrotechnics Seminar (2001), 28th, 781-795
 PUBLISHER: Defence Science & Technology Organisation, Pyrotechnics Group
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB To achieve higher burning rates with rocket propellants some batches have been formulated, for which the main ingredients are (1) the energetic plasticizers GAP-A (short chain GAP with azide end groups), TMETN (trimethylol-ethane trinitrate), and BTTN (1,2,3-butanetriol trinitrate), (2) the energetic substances ammonium perchlorate (AP) and . epsilon.-CL20 (.epsilon.-nitro, -HNIW, hexanitro-hexaza-1,3,4,7,8,10-wurtzitane, crystd. in .epsilon.-nitro-phase). The binder was GAP-N100. From the point of view of stability and ageing, the interesting fact is that the formulations contain none of the typical stabilizers for the nitric acid ester components TMETN and BTTN, although their contents range up to 21 mass %. One reason for doing so is to increase the content of the high energy ingredients. To assess basic stability, a series of tests and investigations were performed. These are the autodetonation temp. test (AIT), Dutch mass loss test (DMLT) and vacuum stability test (VST). To investigate ageing, two measurement quantities are used: mass loss as function of time at the temp. of 70, 80, and 90.degree., and heat generation rate as function of time at 70, 80, and 85.degree.. The evaluation of the measurements is based on reaction kinetic models.
 IT 135285-90-4, CL 20
 RL: TEM (Technical or engineered material use); USES (Uses)
 (ageing and service time period assessment of solid rocket propellant formulations contg. .epsilon.-CL20, ammonium perchlorate and energetic plasticizers)
 RN 135285-90-4 CAPLUS
 CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD.

L10 ANSWER 5 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 2002:605647 CAPLUS
 DOCUMENT NUMBER: 138:41502
 TITLE: On the kinetics and mechanism of phase transformations in hexanitrohexaazaisowurtzitane. the role of water, microstraining and dislocations
 AUTHOR(S): Chukanov, N. V.; Raevskii, A. V.; Golovina, N. I.; Aldoshin, S. M.; Korsounskii, B. L.; Nedelko, V. V.; Dubikhin, V. V.; Volk, F. I.; Kushnarenko, I. A.
 CORPORATE SOURCE: Institute of Problems of Chemical Physics, Moscow Region, Chernogolovka, 142432, Russia
 SOURCE: International Annual Conference of ICT (2002), 33rd(Energetic Materials), 105/1-105/12
 PUBLISHER: Fraunhofer-Institut fuer Chemische Technologie
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Kinetics and mechanisms of phase transformations in the crystals of . epsilon.- and .alpha.-modifications of hexanitrohexaazaisowurtzitane were investigated by using optical microscopy, IR spectroscopy, calorimetry and thermogravimetry. The role of water and dislocations at initial stages of the processes is discussed. After completion of the induction period, the phase transition . epsilon.-. .alpha.-. .gamma.-. In large crystals is controlled by mech. strains and is accompanied by mech. stimulated chem. decompos. in the front of the phase transition wave.
 IT 135285-90-4, Hexanitrohexaazaisowurtzitane.
 RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses)
 (effects of water, microstraining and dislocations on kinetics and mechanism of phase transformations in hexanitrohexaazaisowurtzitane)
 RN 135285-90-4 CAPLUS
 CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

✓ L10 ANSWER 6 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 2002:540857 CAPLUS
 DOCUMENT NUMBER: 137:372230
 TITLE: Kinetic description of mass loss data for the assessment of stability, compatibility and aging of energetic components and formulations exemplified with .epsilon.-CL20

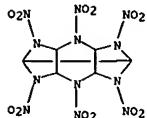
AUTHOR(S): Bohn, Manfred A.
 CORPORATE SOURCE: Fraunhofer-Institut für Chemische Technologie (ICT), Pfinztal, D-76318, Germany
 SOURCE: Propellants, Explosives, Pyrotechnics (2002), 27(3), 125-135
 CODEN: PEPYD5; ISSN: 0721-3115
 PUBLISHER: Wiley-VCH Verlag GmbH
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB The efficiency of the assessment and of the development of energetic materials can be increased by modeling stability, compatibility, aging and thermal decompr. of the used components and formulations. All four terms have in common that chem. reactions are the dominating processes, besides for example migration of mobile components. These chem. reactions are only in part controlled by thermodyn. to a great extent they are controlled kinetically. Kinetic models are formulated and used for mass loss measurements with isothermally operated ovens and TGA (thermogravimetric anal.). The models include autocatalytic decompr. and evapn. of decompr. of a minor component beside a main component. A formulation of a general bimol. reaction in terms of mass loss is useful in compatibility studies. Approxns. and simplifications of the autocatalytic models are discussed. The shown applications include new data on hexanitrohexamethyisowurtzitane crystal, in .epsilon.-phase (.epsilon.-HNW .epsilon.-CL20) and rocket propellant formulations of type HFK contg. .epsilon.-CL20 as main component. The kinetic data for the decompr. of .epsilon.-CL20 are given and discussed with data from literature.

IT 135285-90-4, CL-20
 RL: TEM (Technical or engineered material use); USES (Uses) (kinetic description of mass loss data for assessment of stability and compatibility and aging of energetic components and formulations)

RN 135285-90-4 CAPLUS

CN 5,2,6-(iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

✓ L10 ANSWER 6 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

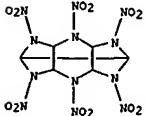
✓ L10 ANSWER 7 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 2002:510118 CAPLUS
 DOCUMENT NUMBER: 137:297021

TITLE: Morphology prediction and simulation of high energy explosives
 AUTHOR(S): Han, Yao-Chung; Lee, Woei-Shyong; Lin, Chiu-Hsiung
 CORPORATE SOURCE: Department of Applied Chemistry, Chung Cheng Institute of Technology, National Defense University, Taiwan
 SOURCE: Huayao Jishu (2002), 18(1), 39-61
 CODEN: HJISE2; ISSN: 1013-767X
 PUBLISHER: Society of Explosives and Propellants
 DOCUMENT TYPE: Journal
 LANGUAGE: Chinese
 AB The aim of this study is to simulate the dynamic crystal morphol. of HNW and ONC, the advanced high-energy explosives. The UFF, the DREIDING and the COMPASS mol. force fields, resp., assocd. with Bravais-Friedel-Donnay-Harker (BFDH) and attachment habit theories were used in the mol. simulations. The computational results of the attachment and the slice energies of the crystal primary faces have shown that the .epsilon.-HNW explosive has less attachment energies and much easier to explode so that it can be used as the warhead's main charge for military purposes. The predictions of the slice energies have concluded that the thermal stability of the ONC explosive is higher than that of the HNW explosive. The packing d. of the ONC explosive is 2.111 kg/m3, which was estd. using the COMPASS mol. force field and was the highest value among the synthesized explosives.

IT 135285-90-4, HNW
 RL: PEP (Properties); TEM (Technical or engineered material use); USES (Uses) (simulation of dynamic crystal morphol. of high energy explosives)

RN 135285-90-4 CAPLUS

CN 5,2,6-(iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



✓ L10 ANSWER 8 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 2002:487940 CAPLUS
 DOCUMENT NUMBER: 137:65360

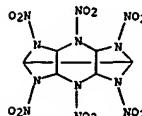
TITLE: Preparation of low-energy-initiated CL-20 explosive by coating of crystals with polymeric binders
 INVENTOR(S): Chan, May L.; Bui-Dang, Que Thinhoc; Hennings, George N.; Reynolds, Thomas Lee; Reynolds, Richard Kent; Ladika, Michael Damon
 PATENT ASSIGNEE(S): USA
 SOURCE: U.S. Pat. Appl. Publ., 6 pp., Division of U. S. Ser. No. 513,035.
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE
 US 2002079030 A1 20020627 US 2001-2594 20011205
 PRIORITY APPLN. INFO.: US 2000-513035 A3 20000225
 AB An explosive suitable for low-energy initiation is prepd. by coating .epsilon.-CL-20 crystals (1-5 .mu.m size) with 1-3 wt.% of a polymeric binder. The polymer binder is selected from polyethyl acrylate, Et acrylate-Bu acrylate copolymer, acrylic polystyrene resin, fluoropolymers, vinyl acetate-ethylene copolymer, vinyl chloride-vinyl acetate copolymer, ethylene-vinyl chloride copolymer, acrylic polymers, polyester-polyurethanes, vinyl acetate-dibutyl maleate copolymer, vinyl acetate-dibutyl maleate-acrylic terpolymer, styrene-butadiene-itaconic acid copolymer, vinylidene chloride-Me methacrylate-acrylonitrile copolymer, vinyl acetate-Bu acrylate copolymer, polyvinyl versatate, and vinylpyrrolidone-styrene copolymer. The explosive is coated by either a slurry method or by using a nonaq. liq. to suspend CL-20 and adding the polymer binder. Such explosives are useful in the fabrication of exploding foil initiators for military ordnance.

IT 135285-90-4, CL-20
 RL: PEP (Physical, engineering or chemical process); PYP (Physical process); TEM (Technical or engineered material use); PROC (Process); USES (Uses) (coating of, prepn. of low-energy-initiated CL-20 explosive by coating of crystals with polymeric binders)

RN 135285-90-4 CAPLUS

CN 5,2,6-(iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



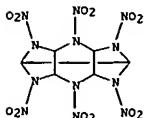
ANSWER 9 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2001:618703 CAPLUS
DOCUMENT NUMBER: 135:290896

TITLE: Theoretical studies on the structures and properties of hexanitrohexaazaisowurtzitane
AUTHOR(S): Zhang, Ji; Xiao, He-Ming; Ji, Guang-Pu
CORPORATE SOURCE: Dep. Chem., Nanjing Univ. of Science and Technol., Nanjing, 210094, Japan
SOURCE: Russ. Xuebao (2001), 59(8), 1265-1271
CODEN: HXHPA4; ISSN: 0567-7351
PUBLISHER: Kexue Chubanshe
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
AB The mol. geometries, electronic structures, IR spectra and thermodyn. properties at 298-1000 K range of α , γ , β , and ϵ -conformations of hexanitrohexaazaisowurtzitane (HNW) are calcd. by using ab initio and d. functional theory (DFT) methods at HF/6-31G* and B3LYP/6-31G* level, resp. The results obtained from the two methods have been carefully compared with each other and with the exptl. data. The optimized parameters of geometries are in good agreement with the exptl. values. Compared with the other bonds in HNW, the bond lengths of N-N are longer and Mulliken population of N-N is smaller, which means that the N-N may be the initial bond in pyrolysis and explosion. The obtained IR spectra are also in good accordance with the exptl. results and the av. abs. difference is < 45 cm $^{-1}$. The thermodyn. stability order [ϵ , α , β , γ] predicted from frontier MO energies and their gaps is the same as that measured from expts.

IT 135285-90-4, Hexanitrohexaazaisowurtzitane
RL: PEP (Physical, engineering or chemical process); PRP (Properties); TEM (Technical or engineered material use); PROC (Process); USES (Uses)
(therm. data, structures and properties of hexanitrohexaazaisowurtzitane)

RN 135285-90-4 CAPLUS

CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



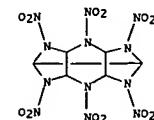
ANSWER 10 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2001:605162 CAPLUS
DOCUMENT NUMBER: 135:325421

TITLE: Solvent effects on the morphology of ϵ -CL-20 crystals
AUTHOR(S): Thome, Volker; Kemps, Paul Bernd; Herrmann, Michael
CORPORATE SOURCE: Fraunhofer ICT, Berghausen, 76327, Germany
SOURCE: International Annual Conference of ICT (2001), 32nd(Energetic Materials), 157/1-157/7
CODEN: IACIEQ; ISSN: 0722-4087
PUBLISHER: Fraunhofer-Institut fuer Chemische Technologie
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A no. of solvents were tested on influencing the morphol. of ϵ -CL-20 crystals. The examples of diisopropyl ether, Me iso-Bu ketone, nitrobenzene and H2O show that different morphologies of ϵ -CL-20 are found after recrystn. Solvents affect crystal growth of CL-20 from soln. and change the morphologies of ϵ -CL-20. This fact is very important for handling CL-20 like filtrating, grinding or storage, because the mech. stability depends on the shape of the crystals. X-ray diffraction patterns of the crystals were analyzed with Rietveld refinement to find out the texture of the faces and the preferred growth directions of the crystals. SEM pictures show that in some cases the blocking of energetically favorable sites by solvent mols. creates odd-looking morphologies.

IT 135285-90-4, CL-20
RL: PRP (Properties)
(solvent effects on morphol. of ϵ -CL-20 crystals)

RN 135285-90-4 CAPLUS

CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 11 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2001:605158 CAPLUS
DOCUMENT NUMBER: 135:259344

TITLE: Stability and service time period assessment of novel solid rocket propellant formulations containing CL20, AP and energetic plasticizers
AUTHOR(S): Bohn, Manfred A.; Eisele, Siegfried
CORPORATE SOURCE: Fraunhofer-Institut fur Chemische Technologie (ICT), Pfingstal-Berghausen, D-76318, Germany
SOURCE: International Annual Conference of ICT (2001), 32nd(Energetic Materials), 152/1-152/13
CODEN: IACIEQ; ISSN: 0722-4087
PUBLISHER: Fraunhofer-Institut fuer Chemische Technologie
DOCUMENT TYPE: Journal
LANGUAGE: German

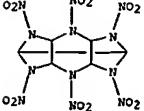
AB To achieve higher burning rates with rocket propellants some batches were formulated, for which the main ingredients are the energetic plasticizers GAP-A, THETN (trimethylolethane trinitrate) and BTTN (1,2,3-butanetricol trinitrate), the energetic substances ammonium perchlorate and ϵ -CL20 (ϵ -CL-20). The binder was GAP-N100. From the view of stability, the interesting fact is that the formulations contain no typical stabilizer for the nitric acid ester components THETN and BTTN, although their contents range 1toreq. 21 mass%. One reason to do this is to increase the content of the high energy substances. To assess the stability and aging a series of tests and investigations was performed. These were Dutch Mass Loss Test, Vacuum Stability Test, mass loss as function of time at the temps. of 80 and 90.degree., and heat generation rate measurements as function of time at 80.degree. with the Thermal Activity Monitor of Thermometric AB, Sweden. The evaluation of the measurements is based on kinetic models.

IT 135285-90-4

RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses)
(stability and service time period assessment of novel solid rocket propellant formulations contg. CL20, AP, and energetic plasticizers)

RN 135285-90-4 CAPLUS

CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 12 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2001:605115 CAPLUS
DOCUMENT NUMBER: 135:311219

TITLE: Phase transformations in hexanitrohexaazaisowurtzitane
AUTHOR(S): Chukanov, N. V.; Golovina, N. I.; Nedelko, V. V.; Dubikhin, V. V.; Voschikova, S. A.; Anan'ina, O. A.; Larikova, T. S.; Nazin, G. M.; Aldoshin, S. M.; Korsounskii, B. L.; Volk, F.

CORPORATE SOURCE: Institute of Problems of Chemical Physics, Russian Academy of Sciences, Chernogolovka, 142432, Russia
SOURCE: International Annual Conference of ICT (2001), 32nd(Energetic Materials), 101/1-101/9
CODEN: IACIEQ; ISSN: 0722-4087

PUBLISHER: Fraunhofer-Institut fuer Chemische Technologie
DOCUMENT TYPE: Journal
LANGUAGE: English

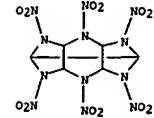
AB Using IR spectroscopy, calorimetry, and x-ray anal. the structure and phase transitions of α - and ϵ - ϵ -modifications of hexanitrohexaazaisowurtzitane into γ -form were studied. The transition α \rightarrow ϵ \rightarrow γ proceeds with self-acceleration. Apparently, this is caused by topochem. nature of the process, including nucleation and frontal propagation. The poor reproducibility of the results is characteristic for the transition ϵ \rightarrow γ . In polycryst. sample. The process has essentially discrete nature, which may be explained by the dependence of the ability of the crystals to undergo phase transition on their morphol., particularly, on the defects in the crystals. Cooperative effect is characteristic for this process. This effect is caused by the ability of phase transition in one crystal to induce the resp. transitions in the whole cluster of adjacent crystals.

IT 135285-90-4, Hexanitrohexaazaisowurtzitane

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(crystal structure and phase transition of)

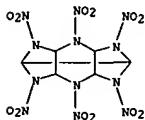
RN 135285-90-4 CAPLUS

CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



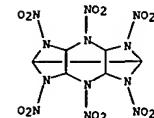
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

✓ ANSWER 13 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 2001:476854 CAPLUS
 DOCUMENT NUMBER: 135:228932
 TITLE: Thermal decomposition of various modifications of hexanitrohexaazaisowurtzitane
 AUTHOR(S): Nedelko, V. V.; Chukanov, N. V.; Golovina, N. I.; Korsunskii, B. L.; Larikova, T. S.; Volk, F.
 CORPORATE SOURCE: Institute of Problems of Chemical Physics, Russian Academy of Sciences, Chernogolovka, 142432, Russia
 SOURCE: New Trends in Research of Energetic Materials, Proceedings of the Seminar, 4th, Pardubice, Czech Republic, Apr. 11-12, 2001 (2001), 257-263.
 Editor(s): Zeman, Svatopluk. University of Pardubice, Pardubice, Czech Rep.
 CODEN: 69BKIC
 DOCUMENT TYPE: Conference
 LANGUAGE: English
 AB The thermal decompr. of .alpha.-, .beta.-, .gamma.-, and .epsilon.-hexanitrohexaazaisowurtzitane (HNW) is investigated by thermogravimetry, IR-spectroscopy, optical microscopy and X-ray diffractometry. At the earliest stages of decompr. (10req. 0.1%) .alpha.-, .beta.-, and .epsilon.-HNW undergo the thermal phase transitions into .gamma.-form. The kinetics of decompr. depends on the particle size and crystal morphol. Decompr. kinetic law of a HNW polymorph is detd. by its crystal nature. Even the very small quantities of water in .epsilon.-HNW (up to 0.1 wt. %) det. the structure of crystal and cause the growth of the elementary cell parameters. This phenomenon affects the decompr. kinetics.
 IT 135285-90-4, Hexanitrohexaazaisowurtzitane
 RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses)
 (detn. of thermal decompr. of various modifications of hexanitrohexaazaisowurtzitane by thermogravimetry and IR-spectroscopy and optical microscopy and X-ray diffractometry)
 RN 135295-90-4 CAPLUS
 CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

✓ ANSWER 14 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 2001:285136 CAPLUS
 DOCUMENT NUMBER: 134:369069
 TITLE: New high explosive - polycyclic nitramine hexanitrohexaazaisowurtzitane (HNW, CL-20)
 AUTHOR(S): Andelkovic-Lukic, Mirjana
 CORPORATE SOURCE: Tehnicki opitni centar, Belgrade, 11000, Yugoslavia
 SOURCE: Naucno-Tehnicki Preleg (2000), 50(6), 60-64
 CODEN: NPGLA7; ISSN: 0350-0667
 PUBLISHER: Vojnotehnicki Institut VJ
 DOCUMENT TYPE: Journal
 LANGUAGE: Serbian
 AB Physico-chem. and detonation properties of a new high explosive are presented and compared with octogen. CL-20 exists in four cryst. forms, stable at different temps. Only the .epsilon.- and the .beta.-form are used in exploitation. CL-20 has better detonation properties than octogen, higher d. and detonation rate but lower impact and friction sensitivity (of the PETN class). The CL-20 m.p. is lower than in octogen, 240 degrees.
 IT 135285-90-4, CL-20
 RL: PRP (Physical, engineering or chemical process); PRP (Properties); TEM (Technical or engineered material use); PROC (Process); USES (Uses)
 (detonation properties of CL-20)
 RN 135285-90-4 CAPLUS
 CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



✓ ANSWER 15 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 2001:279522 CAPLUS
 DOCUMENT NUMBER: 134:282928
 TITLE: Water slurry-coating method for manufacture of pressable and extrudable CL-20-based explosive formulations
 INVENTOR(S): Lee, Kenneth E.; Hatch, Robert L.; Braithwaite, Paul
 PATENT ASSIGNEE(S): Cordant Technologies Inc., USA
 SOURCE: U.S., 9 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

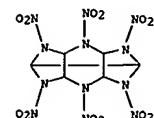
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|------------|
| US 6217799 | BI | 20010417 | US 1998-166843 | 19981006 |
| PRIORITY APPLN. INFO.: | | | US 1997-61236P | P 19971007 |

 AB Pressable or extrudable explosive formulations based on CL-20 are prep'd. by a water slurry method consisting of (1) prep'g. an aq. dispersion of CL-20 (.epsilon.-polymorph), (2) mixing into the dispersion a plasticizer, a lacquer contg. a non-energetic binder, and a solvent, and (3) agitating the slurry and removing the solvent to form coated granules. The mixing and agitating steps are carried out at a sufficiently low temp., and the solvent is present at a suitable low temp., such as to avoid polymorph conversion of the .epsilon.-polymorph of CL-20. The coated granules consist of 85-96 wt. % CL-20, and may also contain a stabilizer (selected from diphenylamine and N-alkylnitroanilines). The formulation can be formed into explosive grains suitable for ordnance, such as grenades, land mines, missile warheads, and demolition explosives.
 IT 135285-90-4, CL-20
 RL: PRP (Physical, engineering or chemical process); TEM (Technical or engineered material use); PROC (Process); USES (Uses)
 (explosives; water slurry-coating method for manuf. of pressable and extrudable CL-20-based explosive formulations)
 RN 135285-90-4 CAPLUS
 CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

✓ ANSWER 16 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 2001:69500 CAPLUS
 DOCUMENT NUMBER: 134:282873
 TITLE: Study on decomposition and impact sensitivity of .epsilon.-hexanitrohexaazaisowurtzitane in three particle sizes
 AUTHOR(S): Xu, Yongjiang; Jin, Shaohua; Ou, Yuxiang; Song, Quancai
 CORPORATE SOURCE: Beijing Institute of Technology, Beijing, 100081, Peop. Rep. China
 SOURCE: Huozhayao Xuebao (2001), 24(1), 47-48, 46
 PUBLISHER: Zhongguo Bingqi Gongye Di-204 Yanjiusuo
 DOCUMENT TYPE: Journal
 LANGUAGE: Chinese
 AB The thermal decompr. of .epsilon.-hexanitrohexaazaisowurtzitane (.epsilon.-HNW) in three particle sizes was studied by DTA, and the formal kinetic parameters E and A were obtained. The impact sensitivity of .epsilon.-HNW corresponding to particle sizes was detd. The effect of particle size on the formal kinetic parameters and impact sensitivity of .epsilon.-HNW was discussed.
 IT 135285-90-4
 RL: PRP (Physical, engineering or chemical process); PRP (Properties); TEM (Technical or engineered material use); PROC (Process); USES (Uses)
 (decompr. and impact sensitivity of .epsilon.-hexanitrohexaazaisowurtzitane in three particle sizes)
 RN 135285-90-4 CAPLUS
 CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



ANSWER 17 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2001:45351 CAPLUS
DOCUMENT NUMBER: 134:133763

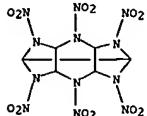
AUTHOR(S): Zhang, Ji Xiao, Hui Yang, Gong, Xue-dong, Li, Jin-shan
CORPORATE SOURCE: Department of Chemistry, Nanjing University of Science and Technology, Nanjing, 210094, P.eop. Rep. China
SOURCE: Henneng Cailliau (2001), 8(4), 149-154
PUBLISHER: Henneng Cailliau Bianjibu
DOCUMENT TYPE: Journal
LANGUAGE: Chinese

AB The quantum-chem. UMF-SCF-PM3 MO method was employed to calc. the pyrolysis initiation reactions of .alpha., .beta., .gamma., .epsilon. and .delta. polymorphs of hexanitrohexaazaisowurtzitane in gas phase. Their transition states, activation energies, and potential energy curves have been obtained. The changes of the geometries, energies and at. charges over these reactions are revealed. The mechanism of pyrolysis initiation reaction of titled compd. is similar to that of usual non-caged nitramine explosives. In addn., the relation between the activation energy and the impact sensitivity is also discussed.

IT 135285-90-4, Hexanitrohexaazaisowurtzitane
RL: PEP (Physical, engineering or chemical process); PRP (Properties); TEM (Technical or engineered material use); PROC (Process); USES (Uses) (anal. of pyrolysis initiation reactions of hexanitrohexaazaisowurtzitane polymorphs in gas phase)

RN 135285-90-4 CAPLUS

CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



L10 ANSWER 18 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 18 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2000:832052 CAPLUS
DOCUMENT NUMBER: 134:6628

AUTHOR(S): Nedelko, V. V.; Chukanov, N. V.; Rasevskii, A. V.; Korsoskii, B. L.; Larkova, T. S.; Kolesova, O. I.; Volk, F.
CORPORATE SOURCE: Institute of Problems of Chemical Physics, Russian Academy of Sciences, Chernogolovka, 142432, Russia
SOURCE: Propellants, Explosives, Pyrotechnics (2000), 25(5), 255-259
CODEN: PEPYD5; ISSN: 0721-3115

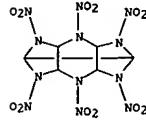
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The thermal decomp. kinetics of different polymorphs of CL-20 (.alpha., .gamma., and .epsilon.) was investigated by thermogravimetry, IR spectroscopy, and optical and electronic microscopy. The reactions proceed with self-acceleration and can be described by a kinetic law of first order with autocatalysis. Already at the earliest stages of decompn. (.10req. 1t) phase transitions take place from .alpha. .fwdrw. .gamma. and from .epsilon. .fwdrw. .gamma. For this reason the obsd. decompn. is related to the decompn. of .gamma.-CL-20. On the other hand, the kinetics of decompn. depends on the initial polymorphic state, so that the thermal decomp. increases in the series: .alpha. < .gamma. < .epsilon.. Expts. with different samples of .alpha.-CL-20 demonstrate that different rates of decompn. are obsd. for the same polymorph depending on the mean size and the size distribution of the crystals and their morphol. features. In some cases the thermal stability of .alpha.-CL-20 can be increased by previous annealing. The thermal decomp. of CL-20 is purely a solid-state process. Microscopical and spectroscopic anal. of the condensed CL-20 decompn. product (formed after prolonged heating at high temp.) show that it has a network structure and consists mainly of carbon and nitrogen.

IT 135285-90-4, Hexanitrohexaazaisowurtzitane

RL: RCT (Reactant); TEM (Technical or engineered material use); RACT (Reactant or reagent); USES (Uses) (comparative anal. of thermal decompn. kinetics of polymorphs of hexanitrohexaazaisowurtzitane)

RN 135285-90-4 CAPLUS

CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



ANSWER 19 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2000:581210 CAPLUS

DOCUMENT NUMBER: 133:195549
TITLE: Polymorphism and solubility of CL20 in plasticisers and polymers

AUTHOR(S): Torry, Simon; Cunliffe, Anthony
CORPORATE SOURCE: DERA, Kent, TN14 7BF, UK
SOURCE: International Annual Conference of ICT (2000), 31st(Energetic Materials), 107/1-107/12
CODEN: IACIEQ; ISSN: 0722-4087

PUBLISHER: Fraunhofer-Institut fuer Chemische Technologie
DOCUMENT TYPE: Journal
LANGUAGE: English

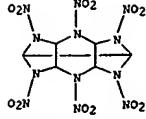
AB The most powerful com. available explosive, 2,4,6,8,10,12-hexanitrohexaazaisowurtzitane (CL20) can exist in at least 4 phases. The preferred polymorph is the .epsilon.-phase as it is morphol. stable at room temp. and has the highest d. of the CL20 polymorphs. The CL20 solv. and the rate of polymorph conversion at various temps. in different plasticizers and polymers were investigated. Solv. was measured using variable temp. proton NMR spectroscopy. The rate of polymorph conversion was quantified by partial least squares anal. of IR spectroscopy data. CL20 polymorph conversion was found to be a complex process. There was evidence that 1:1 mixes of .epsilon.- and .gamma.-CL20 obeyed Ostwald's rule of stages. At temps. above the .epsilon.- to .gamma.-phase transition, the metastable .epsilon.-polymorph was formed in excess before it converted into the stable .gamma.-phase. The .epsilon.- to .gamma.-phase transition temp. was estd. to be 56.5 +/- 1.5 degrees C.

IT 135285-90-4, CL20

RL: PEP (Physical, engineering or chemical process); PRP (Properties); TEM (Technical or engineered material use); PROC (Process); USES (Uses) (polymorphism and solv. of CL20 in plasticizers and polymers)

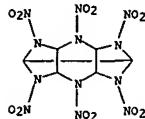
RN 135285-90-4 CAPLUS

CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

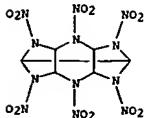
X ANSWER 20 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 2000:581099 CAPLUS
 DOCUMENT NUMBER: 133:179879
 TITLE: Exploring of interactions of the nitramines HMX and CL20 with components in formulations by computer simulation
 AUTHOR(S): Thome, V.; Kempa, P. B.; Bohn, M. A.
 CORPORATE SOURCE: Fraunhofer-Institut fur Chemische Technologie, ICT, Pfingst-Berghausen, D-76318, Germany
 SOURCE: International Annual Conference of ICT (2000), 31st(Energetic Materials), 63/1-63/19
 CODEN: IACIEQ; ISSN: 0722-4087
 PUBLISHER: Fraunhofer-Institut fuer Chemische Technologie
 DOCUMENT TYPE: Journal
 LANGUAGE: German
 AB The development of a methodical determinative model was discussed for prediction of potential intermol. interactions of candidate energetic formulations, based on semiempirical quantum chem. calcns. The compds. in question were cryst.-beta.-HMX and .epsilon.-CL20; reactive formulation components were the energetic binder GAP (glycidyl azide polymer) and guanidine as a carrier for NH2-groups. Reactive configurations were given to analyze bond length changes for the interactions of .beta.-HMX and .epsilon.-CL20 with GAP and guanidine. For GAP, the representative chain length was used for the simulation. Guanidine was comparably reactive for both HMX cryst. forms, although there was a higher tendency for reaction with .epsilon.-CL20. According to the criteria, GAP and .epsilon.-CL20 showed a high reactivity in comparison with .beta.-HMX. The pos. partial charge of the H atom was on average greater with .epsilon.-CL20 than with .beta.-HMX, in which it was assumed that at least one C atom in the CH-CH-group in .epsilon.-CL20 was more pos., which favored the H-cleavage reaction for .epsilon.-CL20, compared with .beta.-HMX.
 IT 135285-90-4, CL-20
 RL: PRP (Properties)
 (systems; modeling of mol. interactions of nitramines with amine and azide components in energetic formulations)
 RN 135285-90-4 CAPLUS
 CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

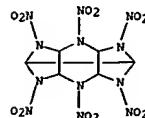
X ANSWER 20 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

X ANSWER 21 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 2000:580918 CAPLUS
 DOCUMENT NUMBER: 133:195542
 TITLE: Comparative investigation of thermal decomposition of various modifications of hexanitrohexaazaisowurtzitane
 AUTHOR(S): Nedelko, V. V.; Chukhov, N. V.; Korsounskii, B. L.; Larikova, T. S.; Volk, F.
 CORPORATE SOURCE: Institute of Problems of Chemical Physics, Russian Academy of Sciences, Moscow Region, 142432, Russia
 SOURCE: International Annual Conference of ICT (2000), 31st(Energetic Materials), 9/1-9/9
 CODEN: IACIEQ; ISSN: 0722-4087
 PUBLISHER: Fraunhofer-Institut fuer Chemische Technologie
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The thermal decompr. of .alpha.-, .gamma.- and .epsilon.-hexanitrohexaazaisowurtzitane (HNIW) has been investigated by manometric, thermogravimetric, IR-spectroscopic and microscopic methods. Kinetic parameters of the reactions have been detd. in terms of the first-order autocatalysis equation. The .alpha.-Form of HNIW has lowered thermal stability as compared with .gamma.- and .epsilon.-forms. The complete thermal phase transitions of .alpha.- and .epsilon.-HNIW polymorphs into .gamma.-HNIW occur already at low decompr. conversions (up to 1%), thus the obsd. difference in the kinetic behavior should be explained by phys. reasons such as morphol., particle size, concn. of defectes.
 IT 135285-90-4, HNIW
 RL: RCT (Reactant); TEM (Technical or engineered material use); RACT (Reactant or reagent); USES (Uses); (comparative investigation of thermal decompr. of various modifications of hexanitrohexaazaisowurtzitane)
 RN 135285-90-4 CAPLUS
 CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

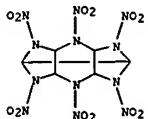
X ANSWER 22 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 2000:353862 CAPLUS
 DOCUMENT NUMBER: 132:349809
 TITLE: New aspects of the impact reactivity of nitramines
 AUTHOR(S): Zeman, Svatopluk
 CORPORATE SOURCE: Department of Theory and Technology of Explosives, University of Pardubice, Pardubice, CZ-532, Czech Rep.
 SOURCE: Propellants, Explosives, Pyrotechnics (2000), 25(2), 66-74
 CODEN: PEPEYD; ISSN: 0721-3115
 PUBLISHER: Wiley-VCH Verlag GmbH
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The impact reactivity ("the first reaction") of nitramines was detd. as the drop energy Ed, required for 50% initiation probability. Relationships were found between the Ed values, on the one hand, and heats of fusion, 15N NMR chem. shifts of azo atoms in reaction centers, parameters of low-temp. thermolysis, and oxygen balances of nitramines studied, on the other. Taking these relationships the Ed values were predicted for 4 nitramines, from which 3 were not synthesized yet. On the basis of the said relationships it was stated that the impact reactivity of nitramine molc. depends on the electronic configuration within their reaction centers and on their conformational stability and intensity of their intermol. interactions. The reaction centers here are the same as in the case of initiation of the nitramines by shock. It is found that .epsilon.-HNIW possesses higher thermal and impact reactivities in comparing with those of .beta.-modification.
 IT 135285-90-4, HNIW
 RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses); (impact reactivity of nitramines)
 RN 135285-90-4 CAPLUS
 CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 62 THERE ARE 62 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

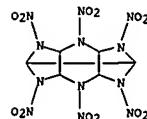
L10 ANSWER 23 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2000:344850 CAPLUS
DOCUMENT NUMBER: 133:45723

TITLE: Quantitative analysis of mixture of .epsilon.-HNIV and .gamma.-HNIV
AUTHOR(S): Gao, Haiyan; Zhang, Yunhong; Yin, Penggang
CORPORATE SOURCE: Fire-retarded Laboratory, Beijing University of Science and Technology, Beijing, 100081, Peop. Rep. China
SOURCE: Huochayao Xuebao (2000), 23(2), 62-63
PUBLISHER: Zhongguo Bingqi Gongye Di-204 Yanjiusuo
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
AB: A method of quant. anal. of mixt. of .epsilon.-HNIV and .gamma.-HNIV by FT-IR was given. The peaks within 832.39-819.312 cm⁻¹ were used as the basis of quant. anal.
IT 135285-90-4, HNIV
RL: PEP (Physical, engineering or chemical process); PRP (Properties); TEM (Technical or engineered material use); PROC (Process); USES (Uses)
(quant. anal. of mixt. of .epsilon.-HNIV and .gamma.-HNIV)
RN 135285-90-4 CAPLUS
CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



L10 ANSWER 24 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2000:344849 CAPLUS
DOCUMENT NUMBER: 133:76151

TITLE: Determination of crystal density of four polymorphs of hexanitrohexaazaisowurtzitane (HNIV)
AUTHOR(S): Ou, Yuming; Xu, Yongjiang
CORPORATE SOURCE: Beijing University of Science and Technology, Beijing, 100081, Peop. Rep. China
SOURCE: Huochayao Xuebao (2000), 23(2), 60-61, 59
PUBLISHER: Zhongguo Bingqi Gongye Di-204 Yanjiusuo
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
AB: The crystal d. (pc and pm) of four polymorphs (.alpha.-HNIV/H2H2O, .beta.-HNIV, .gamma.-HNIV and .epsilon.-HNIV) of HNIV was obtained. The pc was calcd. according to crystal parameters given by X-ray diffractometers. The pm was dstd. according to d. bottle method defined by GB/T772A-97, 401.1. The pc values were 1.992, 1.989, 1.918, and 2.044 g/cm³ resp.; and the pm values were 1.937, 1.983, 1.918, and 2.035 g/cm³ resp. The pc values were 0.055, 0.006, 0, and 0.009 g/cm³ resp., higher than the pm.
IT 135285-90-4, Hexanitrohexaazaisowurtzitane
RL: PEP (Physical, engineering or chemical process); PRP (Properties); TEM (Technical or engineered material use); PROC (Process); USES (Uses)
(detsn. of crystal d. of polymorphs of hexanitrohexaazaisowurtzitane)
RN 135285-90-4 CAPLUS
CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



L10 ANSWER 25 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1999:726251 CAPLUS
DOCUMENT NUMBER: 131:339055

TITLE: Analytical characterization of impurities or byproducts in new energetic materials
AUTHOR(S): Bunte, Gudrun; Pontius, Heike; Kaiser, Manfred
CORPORATE SOURCE: Fraunhofer-Institut für Chemische Technologie (ICT), Pfinztal-Berghausen, D-76327, Germany
SOURCE: Propellants, Explosives, Pyrotechnics (1999), 24(3), 149-155
CODEN: PERYD5; ISSN: 0721-3115

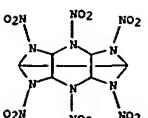
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English

AB: In the last years several new explosives have recently attracted attention as possible alternatives, e.g. for the nitramines RDX and HMX. Hexanitrohexaazaisowurtzitane (HNIV) also known as CL 20 is one of them. Objective of the study was to analyze three different CL 20 samples from different suppliers (.epsilon.-CL 20 from Thiokol, USA and .epsilon.- and .beta.-CL 20 from SNPE, France) with chromatog. and spectroscopic techniques to characterize the chem. and polymorph purity of the materials in order to compare the different samples to each other. From IR-spectroscopic measurements it was dstd. that all three materials have polymorph purities > 95%. To get informations about the chem. purity and possible byproducts or residual solvents the samples were analyzed by HPLC, NMR and GC-MSD. For the last a new technique, the so called solid phase micro exthn., SPME was applied for sample prep. The chem. purity estd. by HPLC anal. was for all CL 20 samples > 96% while the .epsilon.-charge of SNPE had the highest purity (98.3%). From NMR-measurements an acetyl- or formyl-substituted byproduct was identified. From NMR as well as from GC-MSD analyses residual ams. of org. solvents have been detected (ethanol or tetrahydrofuran). Furthermore different spare ams. of other org. components were identified after SPME and characterization with GC-MSD.

IT 135285-90-4, Hexanitrohexaazaisowurtzitane

RL: ANT (Analyte); TEM (Technical or engineered material use); ANST (Analytical study); USES (Uses)
(anal. characterization of impurities or byproducts in energetic materials by using chromatog. and spectroscopic techniques)

RN 135285-90-4 CAPLUS
CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 26 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1999:723022 CAPLUS
DOCUMENT NUMBER: 131:339087

TITLE: Nitration and crystal polymorphism transition in preparation of hexanitrohexaazaisowurtzitane (HNIV) explosive
INVENTOR(S): Duddu, Raja; Dave, Paritosh R.
PATENT ASSIGNEE(S): USA
SOURCE: PCT Int. Appl., 24 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

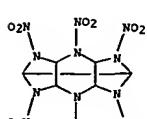
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|------------|
| WO 9957104 | A1 | 19991111 | WO 1999-059167 | 19990427 |
| W: AT, AU, BR, CA, CH, CN, DE, DK, ES, FI, GB, IL, JP, KR, LU, MX, NO, PT, RU, SE, SG, US, ZA | | | | |
| RW: AT, BE, CH, CY, DE, DX, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE | | | | |
| US 6015898 | A | 20000118 | US 1998-71022 | 19980501 |
| AU 9938697 | A1 | 19991123 | AU 1999-38697 | 19990427 |
| US 6160113 | A | 20001121 | US 1999-300988 | 19990428 |
| PRIORITY APPLN. INFO.: | | | US 1998-71022 | A 19980501 |
| | | | WO 1999-059167 | W 19990427 |

AB: The explosive HNIV (hexanitrohexaazaisowurtzitane) is prep'd. by nitration of N-substituted hexaazaisowurtzitane with concd. (i.e., 390%) HNO₃ at >10eq. 75 degrees. (preferably 75-115 degrees.) in which the substrate contains facile leaving groups selected from 1,10eq. 6 H, alkyl, acyl, and acetyl groups, and 1,10eq. 2 alkylaryl or NO₂ (esp. H, MeCO, HCO, PhCH₂, and NO₂) groups. A preferred substrate is tetracyclodiformylisowurtzitan e. The process includes polymorphic conversion of HNIV product (.alpha.-, .beta.-, and .gamma.-) to the .epsilon.-crystal form comprises prep'g. the soln. of HNIV with acetic acid and adding a very small amt. of .epsilon.-HNIV seed crystals, and ptg. .epsilon.-HNIV from the soln.

IT 135285-90-4#

RL: IMP (Industrial manufacture); PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation)
(nitration and crystal polymorphism transition in prep'n. of hexanitrohexaazaisowurtzitane (HNIV) explosive)

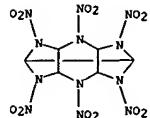
RN 135285-90-4 CAPLUS
CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 26 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

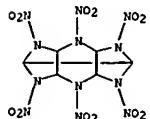
L10 ANSWER 27 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1999:454904 CAPLUS
DOCUMENT NUMBER: 131:118114
TITLE: Kinetics of thermal decomposition of hexanitrohexaazaisowurtzitane
AUTHOR(S): Korsounskii, Boris; Nedolko, Vadim; Chukanov, Nikita; Larikova, Tatiana; Volk, Fred
CORPORATE SOURCE: Institute of Chemical Physics Research, Chernogolovka, 142432, Russia
SOURCE: International Annual Conference of ICT (1999), 30th, 64/1-64/20
CODEN: IACIEQ; ISSN: 0722-4087
PUBLISHER: Fraunhofer-Institut fuer Chemische Technologie
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The thermal decompn. of the title compd. (HNNW) in solid state and in soln. was studied by thermo-gravimetry, manometry, optical microscopy, and IR. On linear heating (4 K/min, initial wt. 10 mg), wt. loss of HNNW begins at 235 degree.. and self-ignition takes place at 243 degree.. The isothermal decompn. of HNNW in solid state proceeds with a self-acceleration. Kinetics of the reaction is described by the equation of 1st-order autocatalysis. At heating a sample to the exptl. temp., apparently, there is a phase transition .epsilonil., .fudarw., .gammaa., whereas during isothermal gravimetric measurement no phase transition occurs. On isothermal gravimetric measurement the thermal stability of HNNW is much lower than that of HMX. In m-dinitrobenzene soln. the reaction proceeds according to the 1st-order kinetic equation. The rate constants and activation parameters of HNNW thermal decompn. in solid state and in soln. were detd. The reactivity of HNNW in soln. exceeds that of HMX by >2 orders. The volatility of HNNW is much lower than that of HMX. N content ams. to approx. 1/2 of gaseous products of HNNW thermolysis. Thermolysis of HNNW and its ignition at heating are accompanied by formation of a condensed residue. During these processes 3 of 6 NO₂ groups present in a HNNW mol. are lost. The residue contains NH₂ groups and does not contain C=H bonds.
IT 135285-90-4, Hexanitrohexaazaisowurtzitane
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(thermal decompn. of nitrohexaazaisowurtzitane and kinetics thereof)
RN 135285-90-4 CAPLUS
CN 5,2,6-(Iminomethinium)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS

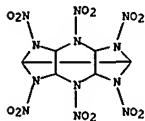
L10 ANSWER 27 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 28 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1999:273151 CAPLUS
DOCUMENT NUMBER: 131:18700
TITLE: Effect of particle size on the thermal decomposition of .vepsilin.-hexanitrohexaazaisowurtzitane
AUTHOR(S): Kim, Jun-Hyung; Yim, Yoo-Jin
CORPORATE SOURCE: Agency for Defense Development, Taejon, 305-600, S. Korea
SOURCE: Journal of Chemical Engineering of Japan (1999), 32(2), 237-241
PUBLISHER: Society of Chemical Engineers, Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The influence of the particle size on the thermal decompn. of .vepsilin.-hexanitrohexaazaisowurtzitane (HNNW) was studied by DSC. The kinetics and mechanism for the decompn. were evaluated using integral methods. The thermal kinetic parameters such as activation energy (E) and pre-exponential factor (A) depend little on the particle size of .vepsilin.-HNNW in the range 4-190 .mu.m, and an AJ model function fits most of the data from the decompn. of the material.
IT 135285-90-4, Hexanitrohexaazaisowurtzitane
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(effect of particle size on thermal decompn. of .vepsilin.-hexanitrohexaazaisowurtzitane)
RN 135285-90-4 CAPLUS
CN 5,2,6-(Iminomethinium)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

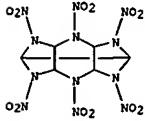
L10 ANSWER 29 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1998:498910 CAPLUS

DOCUMENT NUMBER: 129-110975
TITLE: Characterization of impurities in new energetic materials
AUTHOR(S): Bunte, G.; Pontius, H.; Kaiser, M.
CORPORATE SOURCE: Fraunhofer-Instit. Chemische Technologie, Pfingstal, D-76327, Germany
SOURCE: International Annual Conference of ICT (1998), 29th(Energetic Materials), 148, 1-148.10
CODEN: IACIEQ; ISSN: 0722-4087
PUBLISHER: Fraunhofer-Institut fuer Chemische Technologie
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Three samples of hexanitrohexaazaisowurtzitane (HNIW, CL 20) from different suppliers (. ϵ -epsilon.-CL 20 from Thiokol, USA and . ϵ -epsilon.-CL 20 from SNPE, France) were analyzed with chromatog. and spectroscopic techniques to characterize the chem. and polymorph purity of the materials. To compare the different samples IR-spectroscopic measurements showed that all 3 materials have polymorph purities >95 %. To get information about the chem. purity and possible byproducts or residual solvents the samples were analyzed by HPLC, NMR, and GC-MSD. Solid-Phase Micro Extrn. (SPME) was applied for sample prep. The chem. purity estd. by HPLC anal. was for all CL 20 samples >96 % while the NMR-measurement of SNPE had the highest purity (98.3%). From NMR-measurements a formyl-substituted byproduct was identified. From NMR as well as from GC-MSD analyses residual amt. of org. solvents were detected (ethanol or tetrahydrofuran). Furthermore different trace amt. of other org. components were identified after SPME-treatment and characterization with GC-MSD.
IT 135285-90-4, CL 20
RL: ANX (Analytical matrix); TEM (Technical or engineered material use); ANST (Analytical study); USES (Uses)
(anal. characterization of impurities in)
RN 135285-90-4 CAPLUS
CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



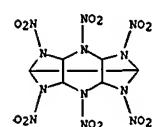
L10 ANSWER 31 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1998:498855 CAPLUS

DOCUMENT NUMBER: 129-138140
TITLE: Fine grinding of explosives
AUTHOR(S): Gerber, P.; Zilly, B.; Teipel, U.
CORPORATE SOURCE: Fraunhofer-Institut Chemische Technologie, Pfingstal, D-76327, Germany
SOURCE: International Annual Conference of ICT (1998), 29th(Energetic Materials), 71, 1-71.12
CODEN: IACIEQ; ISSN: 0722-4087
PUBLISHER: Fraunhofer-Institut fuer Chemische Technologie
DOCUMENT TYPE: Journal
LANGUAGE: German
AB A wet grinding process with a rotor-stator mill was selected for safe grinding of the explosive . ϵ -epsilon.-CL-20 with a mean particle size of 200 . μ m. to produce a narrow particle size distribution and a mean particle size of 5 . μ m. The aq. suspension had a solid concn. of 15 %. The obtained particle size distribution of . ϵ -epsilon.-CL-20 is compared to that of RDX.
IT 135285-90-4, CL-20
RL: PEP (Physical, engineering or chemical process); PRP (Properties); TEM (Technical or engineered material use); PROC (Process); USES (Uses)
(fine grinding of explosives)
RN 135285-90-4 CAPLUS
CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



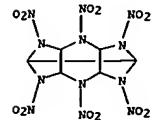
L10 ANSWER 30 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1998:498907 CAPLUS

DOCUMENT NUMBER: 129-138146
TITLE: Thermal behavior and stability of HNIW (CL20)
AUTHOR(S): Loebbecke, S.; Bohn, M. A.; Pfeil, A.; Krause, A.
CORPORATE SOURCE: Fraunhofer-Instit. Chemische Technologie, Pfingstal, D-76327, Germany
SOURCE: International Annual Conference of ICT (1998), 29th(Energetic Materials), 145, 1-145.15
CODEN: IACIEQ; ISSN: 0722-4087
PUBLISHER: Fraunhofer-Institut fuer Chemische Technologie
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The thermal stability, phase behavior, and decompr. of the explosive . ϵ -epsilon.-CL-20, . ϵ -epsilon.-NO2, . ϵ -epsilon.-N2O, and . ϵ -epsilon.-NCO were studied. At >164 degree. irreversible transition to the . γ -polymorph was obstd. which is accompanied by an increase of vol. Differential scanning calorimetry and differential thermogravimetry indicate a 2-step decompr. at >210 degree. The evolution of gaseous decompr. products was monitored by rapid scan FTIR spectroscopy. The main products are CO2, NO2, N2O, and HCN. In addn., a solid residue remains whose IR spectrum is given. A mass loss due to decompr. was also obstd. below 210 degree.. Kinetic calcs. show this low-temp. decompr. reaction to be of 1st order and autocatalytic.
IT 135285-90-4, CL-20
RL: PEP (Physical, engineering or chemical process); PRP (Properties); TEM (Technical or engineered material use); PROC (Process); USES (Uses)
(thermal behavior and stability of HNIW (CL 20))
RN 135285-90-4 CAPLUS
CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



L10 ANSWER 32 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1998:60143 CAPLUS

DOCUMENT NUMBER: 128-117010
TITLE: Sensitivity and spectroscopic properties of the .beta.- and . ϵ -epsilon.-polymorphs of HNIW
AUTHOR(S): Ostmark, Henric; Bergman, Helena; Sjoberg, Per
CORPORATE SOURCE: Natl. Defence Res. Establishment, Sundbyberg, S-17290, Swed.
SOURCE: Proceedings - International Symposium on Energetic Materials Technology, Phoenix, 1995 (1995), 76-81. American Defense Preparedness Association: Arlington, Va.
CODEN: 65NDAP
DOCUMENT TYPE: Conference
LANGUAGE: English
AB A study was presented of the sensitivity and spectroscopic properties of the .beta.- and . ϵ -epsilon.-polymorphs of HNIW (2,4,6,8,10,12-hexanitrohexaazaisowurtzitan). The thermal stability was studied using DSC technique which was also used to measure the activation energy and the frequency factor. The sensitivity was examd. by drop-wt. test and friction test. The drop-wt. test points to a higher sensitivity for the . ϵ -epsilon.-polymorph (18 cm for . ϵ -epsilon.- vs. 67 cm for the .beta.-polymorph), whereas the sensitivity to friction was similar for the two polymorphs. A HPLC anal. method was developed to analyze HNIW in soln. Mass spectra (electron impact and chem. ionization) for both polymorphs were also given. The best routine method so far for analyzing the polymorphs of HNIW is Fourier-transform IR spectroscopy which was used to distinguish the polymorphs. An alternative to the FTIR method, Fourier-transform Raman spectroscopy (FT Raman spectroscopy), uses only a small amt. of solid samples (a few mg) and was easy to carry out. The FT Raman spectra for the .beta.- and . ϵ -epsilon.-polymorphs of HNIW showed major differences and can thus be used for fingerprinting.
IT 135285-90-4
RL: PEP (Properties); TEM (Technical or engineered material use); USES (Uses)
(sensitivity and spectroscopic properties of .beta.- and . ϵ -epsilon.-polymorphs of HNIW)
RN 135285-90-4 CAPLUS
CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



X 10 ANSWER 33 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1998:38963 CAPLUS

DOCUMENT NUMBER: 128:123816

TITLE: Molecular Packing and NPT-Molecular Dynamics Investigation of the Transferability of the RDX Intermolecular Potential to 2,4,6,8,10,12-Hexanitrohexaazaisowurtzitane

AUTHOR(S): Sorescu, Dan C.; Rice, Betsy M.; Thompson, Donald L. CORPORATE SOURCE: Department of Chemistry, Oklahoma State University, Stillwater, OK, 74078, USA

SOURCE: Journal of Physical Chemistry B (1998), 102(6), 948-952

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

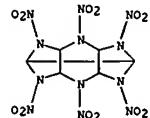
AB The degree to which intermol. potential for the explosive hexahydro-1,3,5-trinitro-1,3,5-s-triazine (RDX) is transferable for predictions of crystal structures (within the approx. of rigid mol.) of a similar chem. system, in this case, polymorphic phases of the 2,4,6,8,10,12-hexanitrohexaazaisowurtzitane (HNIW) crystal was explored. Mol. packing and isothermal-isobaric mol. dynamics calcns. performed with this potential reproduce the main crystallog. features of the .epsilon., .beta., and .gamma.-HNIW crystals. Thermal expansion coeffs. calcld. using the present model predict near isotropic expansion for the .epsilon., and .gamma.-HNIW crystals phases and anisotropic expansion for .beta.-HNIW.

IT 135285-90-4, 2,4,6,8,10,12-Hexanitrohexaazaisowurtzitane

RL: PRP (Properties)
(mol. packing and NPT-mol. dynamics investigation of transferability of RDX intermol. potential to calcn. of crystal structure of hexanitrohexaazaisowurtzitane)

RN 135285-90-4 CAPLUS

CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

X 10 ANSWER 34 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1997:730088 CAPLUS

DOCUMENT NUMBER: 128:5410

TITLE: CL-20 performance exceeds that of HMX and its sensitivity is moderate

AUTHOR(S): Simpson, R. L.; Urtiew, P. A.; Orellas, D. L.; Moody, G. L.; Scribner, K. J.; Hoffmann, D. M.

CORPORATE SOURCE: Energetic Materials Center, University California, Livermore, CA, 94550, USA

SOURCE: Propellants, Explosives, Pyrotechnics (1997), 22(5), 249-255

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The explosive performance of .epsilon.-CL-20 is approx. 14% greater than that of HMX as detd. by cylinder expansion and Ta plate acceleration expts. This makes it the most powerful explosive ever tested at small vol. expansions of the detonation products. In general CL-20 is more sensitive than HMX. However, the sensitivity of CL-20 to 1-dimensional shock loading is similar to HMX.

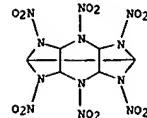
IT 135285-90-4, CL 20

RL: PRP (Properties)

(explosive performance and sensitivity of CL-20 compared with HMX)

RN 135285-90-4 CAPLUS

CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



X 10 ANSWER 35 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1997:570534 CAPLUS

DOCUMENT NUMBER: 127:236415

TITLE: Theoretical calculation on .epsilon.-.Hexanitrohexaazaisowurtzitane structure

AUTHOR(S): Li, Laicai; Yang, Chun CORPORATE SOURCE: Department of Chemistry, Sichuan Normal University, Chengdu, 610066, Peop. Rep. China

SOURCE: Sichuan Shifan Daxue Xuebao, Ziran Kexueban (1997), 20(3), 71-73

CODEN: SDKEEP; ISSN: 1001-8395

PUBLISHER: Sichuan Shifan Daxue

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

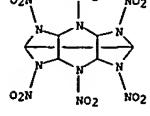
AB The PM3 (MO) method was used to optimize the structure of .epsilon.-HNIW (hexanitrohexaazaisowurtzitane), and the explosive properties of .epsilon.-HNIW were discussed theor.

IT 135285-90-4

RL: PRP (Properties)
(PM3 MO calcn. of structure and properties of .epsilon.-HNIW)

RN 135285-90-4 CAPLUS

CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



X 10 ANSWER 36 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1996:517341 CAPLUS

DOCUMENT NUMBER: 125:200045

TITLE: Shock initiation of an .epsilon.-CL-20-Estane formulation

AUTHOR(S): Tarver, C. M.; Simpson, R. L.; Urtiew, P. A. CORPORATE SOURCE: Lawrence Livermore National Laboratory, Livermore, CA, 94551, USA

SOURCE: AIP Conference Proceedings (1996), 370(Pt. 2, Shock Compression of Condensed Matter--1995), 891-894

CODEN: APFCPS; ISSN: 0094-243X

PUBLISHER: AIP Press

DOCUMENT TYPE: Journal

LANGUAGE: English

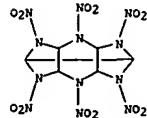
AB The shock sensitivity of a pressed solid explosive formulation, LX-19, contg. 95.2% by wt. .epsilon.-phase 2,4,6,8,10,12-hexanitrohexaazaisowurtzitane (HNIW) and 4.8% Estane binder, was detd. using the wedge test and embedded manganin pressure gauge techniques. This formulation was slightly more sensitive than LX-14, which contains 95.5% HMX and 4.5% Estane binder. The measured pressure histories for LX-19 were very similar to those obtained using several HMX-inert binder formulations. An ignition and growth reactive flow model for LX-19 was developed (using two Jones-Wilkins-Lee equations of state) which differed from those for HMX-inert binder formulations only by a 25% higher hot spot growth rate.

IT 135285-90-4, LX 19

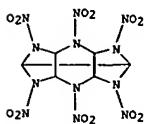
RL: RCT (Reactant); TEM (Technical or engineered material use); RACT (Reactant or reagent); USES (Uses)
(LX 19; flow modeling of shock sensitivity of pressed explosive contg. hexanitrohexaazaisowurtzitane and estane binder)

RN 135285-90-4 CAPLUS

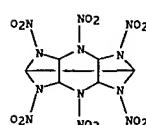
CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



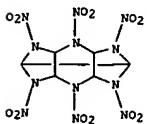
ANSWER 37 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1996:470483 CAPLUS
 DOCUMENT NUMBER: 125:128340
 TITLE: Crystal and molecular structures of .epsilon.-HNIV
 AUTHOR(S): Zhao, Xinqi; Shi, Nizheng
 CORPORATE SOURCE: Department Chemical Engineering, Beijing Institute of Technology, Beijing, 100081, Peop. Rep. China
 SOURCE: Chinese Science Bulletin (1996), 41(7), 574-576
 CODEN: CSBUDF; ISSN: 1001-6538
 PUBLISHER: Science Press
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The title compd. (the polymorph of hexanitrohexaazaisowurtzitane with the highest crystal d.) is monoclinic, space group P21/n, with a 1.3696(7), b 1.2554(6), c 0.8833(4) nm, and β = 111.18(2) degrees; Z = 4, dc = 2.055; R = 0.066, R_w = 0.074 for 2658 reflections. At. coordinates are given. The C-N and C-H bond lengths in the mol. are typical. The nitramine group is essentially in a plane configuration. C-C bond lengths are 0.1575-0.1590 nm.
 IT 135285-90-4, Hexanitrohexaazaisowurtzitane
 RL: PRP (Properties)
 (crystal structure of polymorph of)
 RN 135285-90-4 CAPLUS
 CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



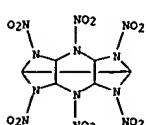
ANSWER 38 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1996:285210 CAPLUS
 DOCUMENT NUMBER: 124:320936
 TITLE: Determination of thermal stabilities of .epsilon.-HNIV and HMX using accelerating rate calorimeter (ARC)
 AUTHOR(S): Wan, Xingzhong; Ou, Yuxiang; Chen, Boron; Feng, Changgen
 CORPORATE SOURCE: Beijing Institute of Technology, Beijing, 100081, Peop. Rep. China
 SOURCE: Proceedings of the Beijing International Symposium on Pyrotechnics and Explosives, 3rd, Beijing, Nov. 6-9, 1995 (1995), 520-525. Editor(s): Yuxiang, Ou. China Ordnance Society: Beijing, Peop. Rep. China.
 CODEN: 62RIAT
 DOCUMENT TYPE: Conference
 LANGUAGE: English
 AB The adiabatic thermal decompn. kinetics of .epsilon.-CL-20 and HMX was studied in an accelerating rate calorimeter. The self-heating rates and the pressure increase rates were measured as function of self-heating temp. The activation energies for the decompn. of these explosives were detd. from the self-heating rates. The onset temp. of the self-heating was always much lower than the corresponding std. deflagration temp. (which was detd. with a std. app.). The temp. of onset of self-heating of .epsilon.-CL-20 was lower than that of HMX.
 IT 135285-90-4
 RL: PRP (Properties)
 (thermal stability and adiabatic thermal decompn. kinetics of HNIV and HMX in accelerating rate calorimeter)
 RN 135285-90-4 CAPLUS
 CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



ANSWER 39 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1996:285182 CAPLUS
 DOCUMENT NUMBER: 124:320934
 TITLE: Study on 100.degree.C heat test of .epsilon.-HNIV
 AUTHOR(S): Zhao, Xinqi; Li, Li; Yang, Zongyun; Yu, Yongzhong
 CORPORATE SOURCE: Beijing Institute of Technology, Beijing, 100081, Peop. Rep. China
 SOURCE: Proceedings of the Beijing International Symposium on Pyrotechnics and Explosives, 3rd, Beijing, Nov. 6-9, 1995 (1995), 312-314. Editor(s): Yuxiang, Ou. China Ordnance Society: Beijing, Peop. Rep. China.
 CODEN: 62RIAT
 DOCUMENT TYPE: Conference
 LANGUAGE: English
 AB Loss in wt. of .epsilon.-HNIV (CL-20) at 100.degree. during two 48-h periods was only 0.02%, and no changes in phys. appearance of the crystals were noted. Neither ignition nor explosion occurred after 300-h heating. The FTIR spectra before and after 300-h heating confirmed that no phase transformation was evident.
 IT 135285-90-4, Hexanitrohexaazaisowurtzitane
 RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses)
 (explosive; thermal stability of)
 RN 135285-90-4 CAPLUS
 CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



ANSWER 40 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1996:255293 CAPLUS
 DOCUMENT NUMBER: 124:293607
 TITLE: Phase transition in HNIV (CL-20) polymorphs and its application in propellants
 AUTHOR(S): Feng, Zengguo
 CORPORATE SOURCE: Beijing Inst. of Technology, Beijing, 100081, Peop. Rep. China
 SOURCE: Binggong Xueba, Huohuangong Fence (1996), 18(1), 46-9, 42
 CODEN: EXHFFP; ISSN: 1004-9193
 PUBLISHER: Zhongguo Bingqi Gongye Di-204 Yanjiuso
 DOCUMENT TYPE: Journal
 LANGUAGE: Chinese
 AB Recently, hexanitrohexaazaisowurtzitane (HNIV; i.e. CL-20) was obsd. to exist in six different polymorphs, from which .alpha., .beta., .gamma., and .epsilon.-polymorphs have been sep'd. and detd. Calcs. for detonation parameters and specific impulse revealed that CL-20 was more energetic than HMX and RDX, but it was remarkably different with respect to phase conversion, thermal stability, and solv. Based on available refs. and exptl. data on RDX and polymorphic changes of ammonium nitrate, some views were suggested about phase transitions in CL-20 polymorphs and its application in propellants.
 IT 135285-90-4
 RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses)
 (phase transition in HNIV polymorphs and application as solid propellants)
 RN 135285-90-4 CAPLUS
 CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



ANSWER 41 OF 47 CAPIUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1996:202406 CAPIUS
DOCUMENT NUMBER: 124:236477

TITLE: Thermal stability of ϵ -HNHAIW at 100.degree.C

AUTHOR(S): Zhao, Xinqi; Li, Li
CORPORATE SOURCE: Sch. Chem. Eng., Materials Sci., Beijing Inst. Technol., Beijing, 100081, Peop. Rep. China

SOURCE: Hanning Cailiao (1995), 3(4), 31-4

CODEN: HACAFQ; ISSN: 1006-9941

PUBLISHER: Hanning Cailiao Bianjibu

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

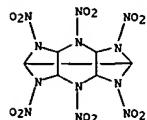
AB Hexanitrohexaazaisowurtzitane (HNHAIW) was heated at 100.degree. for 48.96 and 300 h, resp., with no observable burning or explosion. The crystals had no visible changes in appearance and no crystal configuration transitions identifiable by FT-IR anal. A wt. loss of 0.02% after 96 h heating indicated that the thermal stability of ϵ -HNHAIW was better than that of RDX and HMX.

IT 135285-90-4, Hexanitrohexaazaisowurtzitane

RL: PRP (Properties); (thermal stability of)

RN 135285-90-4 CAPIUS

CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



ANSWER 42 OF 47 CAPIUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1995:507758 CAPIUS
DOCUMENT NUMBER: 123:36618

TITLE: Sensitivity studies of a new energetic formulation
AUTHOR(S): Wilson, W. H.; Forbes, J. W.; Liddiard, T. P.; Doherty, R. M.

CORPORATE SOURCE: Dahlgren Div., Naval Surface Warfare Cent., Silver Spring, MD, 20903-5640, USA

SOURCE: AIP Conference Proceedings (1994), 309(High-Pressure Science and Technology--1993, Pt. 2), 1401-4
CODEN: APCPC5; ISSN: 0094-243X

PUBLISHER: AIP Press

DOCUMENT TYPE: Journal

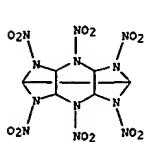
LANGUAGE: English

AB The shock sensitivity of a new pressed formulation, PEXC 19, which is similar to LX-14 but contains CL-20 instead of HMX, was studied. Samples were made from a bimodal particle size distribution of CL-20, ϵ -polymorph and an ethylene-vinyl acetate binder, pressed to an av. 97% of theor. max. d. The material exhibited an anomalous reversal in slope of shock sensitivity vs. input stress. Over a limited stress range near the first reaction threshold, the level of reaction decreased with increasing input stress. Within this range of input shock, it was obstd. that break-off of reaction was delayed, and was concd. near the sample centerline.

IT 135285-90-4, CL-20

RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses); (explosives contg., shock sensitivity of pressed CL20-based explosive formulation)

RN 135285-90-4 CAPIUS
CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



ANSWER 42 OF 47 CAPIUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1995:595376 CAPIUS
DOCUMENT NUMBER: 124:33113

TITLE: Structural identification of hexanitrohexaazaisowurtzitane

AUTHOR(S): Ou, Yuming; Chen, Boren; Jia, Huiping; Pan, Zelin; Xu, Yongjian
CORPORATE SOURCE: College Chem. Eng. Material Sci., Beijing Inst. Technology, Beijing, 100081, Peop. Rep. China

SOURCE: Hanning Cailiao (1995), 3(3), 1-8

CODEN: HACAFQ; ISSN: 1006-9941

PUBLISHER: Hanning Cailiao Bianjibu

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

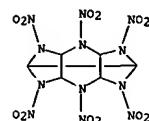
AB The mol. structure of CL-20 synthesized by authors was identified by FTIR, 1H-NMR, 13C-NMR, CIMS, UV, and elemental anal. The four polymorphs (α -, β -, γ -, and ϵ -) of CL-20 was prep'd., and also characterized by FTIR. The characteristic peaks of the polymorphs in the "fingerprint" region (1200-700 cm⁻¹) were in agreement with those reported in literatures. The structure of CL-20 and its four polymorphs were clarified.

IT 135285-90-4, Hexanitrohexaazaisowurtzitane

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); (structural identification of hexanitrohexaazaisowurtzitane and its polymorphs)

RN 135285-90-4 CAPIUS

CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



ANSWER 43 OF 47 CAPIUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1995:507758 CAPIUS
DOCUMENT NUMBER: 123:36618

TITLE: The thermal stability of the polymorphs of hexanitrohexaazaisowurtzitane. Part II

AUTHOR(S): Foltz, M. Frances; Coon, Clifford L.; Garcia, Frank; Nichols, Albert L., III
CORPORATE SOURCE: Lawrence Livermore Natl. Lab., Livermore, CA, 94550, USA

SOURCE: Propellants, Explosives, Pyrotechnics (1994), 19(3), 133-44

CODEN: PEVDUS; ISSN: 0721-3115

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Solid-solid phase transitions in the α -, β -, γ -, and ϵ -polymorphs of 2,4,6,10,12-hexanitrohexaazaisowurtzitane (HNHW) were studied as a function of temp. Techniques used include differential scanning calorimetry (DSC), DTA/thermogravimetric anal. (DTA/TGA), and hot stage microscope anal. Fourier-transform IR spectroscopy (FTIR) was used to identify results of polymorphic conversion. Results corroborate those of Part I [M. Foltz, C. Coon, et al (1994)] that the existence of multiple α -hydrate phases complicates definition of the HNHW pressure-temp. phase diagram. A high-temp. endothermic DSC response was detd. by FTIR spectroscopy to be the β - γ transition, not a conversion to a high-temp. "delta" phase. The role of water in the shifting this conversion to higher temp. was discussed.

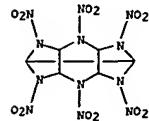
IT 135285-90-4

RL: USES (Uses)

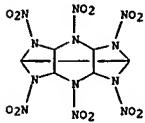
(polymorphs of, thermal stability of)

RN 135285-90-4 CAPIUS

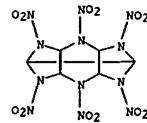
CN 5,2,6-(Iminomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-hexanitro- (9CI) (CA INDEX NAME)



10 ANSWER 45 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1994:326923 CAPLUS
 DOCUMENT NUMBER: 120:326923
 TITLE: Thermal stability of .epsilon.
 .hexanitrohexaazaisowurtzitane in an Estane
 formulation
 AUTHOR(S): Foltz, M. Frances
 CORPORATE SOURCE: Lawrence Livermore Natl. Lab., Livermore, CA, 94550,
 USA
 SOURCE: Propellants, Explosives, Pyrotechnics (1994), 19(2),
 63-9
 CODEN: PEPYD5; ISSN: 0721-3115
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB A change in color and d. during prolonged heating of a formulation contg.
 .epsilon.-hexanitrohexaazaisowurtzitane (HNIV) and Estane 5702
 was investigated by Fourier transform IR spectroscopy. Polymorphic
 impurities were obad. at all stages of prodn. and processing, the nature
 and concn. of which changed with treatment of the material.
 Thermally-induced polymorphic conversion was dtd. to be the cause of the
 decrease in d., whereas the color change was speculated to be the result
 of binder degradn. Sensitivity to impact, friction, and electrostatic
 spark were unchanged.
 IT 135285-90-4, Hexanitrohexaazaisowurtzitane
 RL: USES (Uses)
 (explosives, contg. urethane rubber binder, thermal stability of)
 RN 135285-90-4 CAPLUS
 CN 5,2,6-(Ininomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-
 hexanitro- (9CI) (CA INDEX NAME)



10 ANSWER 46 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1994:248721 CAPLUS
 DOCUMENT NUMBER: 120:248721
 TITLE: The thermal stability of the polymorphs of
 hexanitrohexaazaisowurtzitane. Part I
 AUTHOR(S): Foltz, M. Frances; Coon, Clifford L.; Garcia, Frank;
 Nicholas, Albert L., III
 CORPORATE SOURCE: Lawrence Livermore Natl. Lab., Livermore, CA, 94550,
 USA
 SOURCE: Propellants, Explosives, Pyrotechnics (1994), 19(1),
 19-25
 CODEN: PEPYD5; ISSN: 0721-3115
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Phase transitions in the .alpha., .beta., .gamma., and .epsilon.
 .-polymorphs of 2,4,6,8,10,12-hexanitrohexaazaisowurtzitane (HNIV) were
 studied as a function of temp. In addn., results were presented for
 high-temp. equil. solvation studies coupled with Fourier-transform IR
 spectroscopy for the identification of polymorphic conversion. These
 results were augmented by literature data from differential scanning
 calorimetry, DTA-thermogravimetric anal., and optical hot-stage
 microscopy. The thermodynamic stability of the polymorphs decreased in the
 order: .epsilon. > .gamma. > .alpha.-hydrate > .beta.. with the
 .epsilon.-phase polymorph being the most thermodynamically stable phase
 of HNIV at room temp. The existence of multiple .alpha.-hydrate phases
 complicated the deta. of the equil. pressure-temp. phase diagram of HNIV.
 IT 135285-90-4
 RL: USES (Uses)
 (polymorphs of, phase transitions and thermal anal. and phase diagrams
 of)
 RN 135285-90-4 CAPLUS
 CN 5,2,6-(Ininomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-
 hexanitro- (9CI) (CA INDEX NAME)



10 ANSWER 47 OF 47 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1993:132609 CAPLUS
 DOCUMENT NUMBER: 110:132609
 TITLE: Pressure/temperature phase diagram of
 hexanitrohexaazaisowurtzitane
 AUTHOR(S): Russell, T. P.; Miller, P. J.; Piermarini, G. J.;
 Block, S.
 CORPORATE SOURCE: Nav. Surface Warfare Cent., Silver Spring, MD,
 20901-5000, USA
 SOURCE: Journal of Physical Chemistry (1993), 97(9), 1993-7
 CODEN: JPCHAX; ISSN: 0022-3654
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The five known polymorphs of hexanitrohexaazaisowurtzitane (chem. name:
 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexazatetracyclo[5.5.0.0.5,9.0.3,11]
 dodecane), .alpha., .beta., .gamma., .epsilon., and .zeta., were
 studied by optical polarizing light microscopy (OPLM) and Fourier
 transform IR spectroscopy (FTIR) as a function of temp. and pressure. A
 high-temperature/high-pressure diamond anvil cell specially designed for
 these studies was employed. Four reversible and five unidirectional phase
 transformations were obad. and identified by FTIR spectra. Phase
 boundaries were studied as function of pressure and temp. permitting a
 delineation of the various polymorph stability fields. A pressure/temp.
 reaction/phase diagram for the .gamma. polymorph to 14.0 GPa and temps.
 between -125 and 340 degree. (or to thermal decomp. temps.), is presented.
 The FTIR spectra for all five polymorphs were obtained as functions of
 temp. and pressure. An .alpha. phase with trapped CO2/CO was obad. by
 FTIR. The thermal decomp. temp./pressure parameters were also dtd.
 IT 135285-90-4
 RL: PRP (Properties)
 (pressure-temp. phase diagram of)
 RN 135285-90-4 CAPLUS
 CN 5,2,6-(Ininomethenimino)-1H-imidazo[4,5-b]pyrazine, octahydro-1,3,4,7,8,10-
 hexanitro- (9CI) (CA INDEX NAME)

